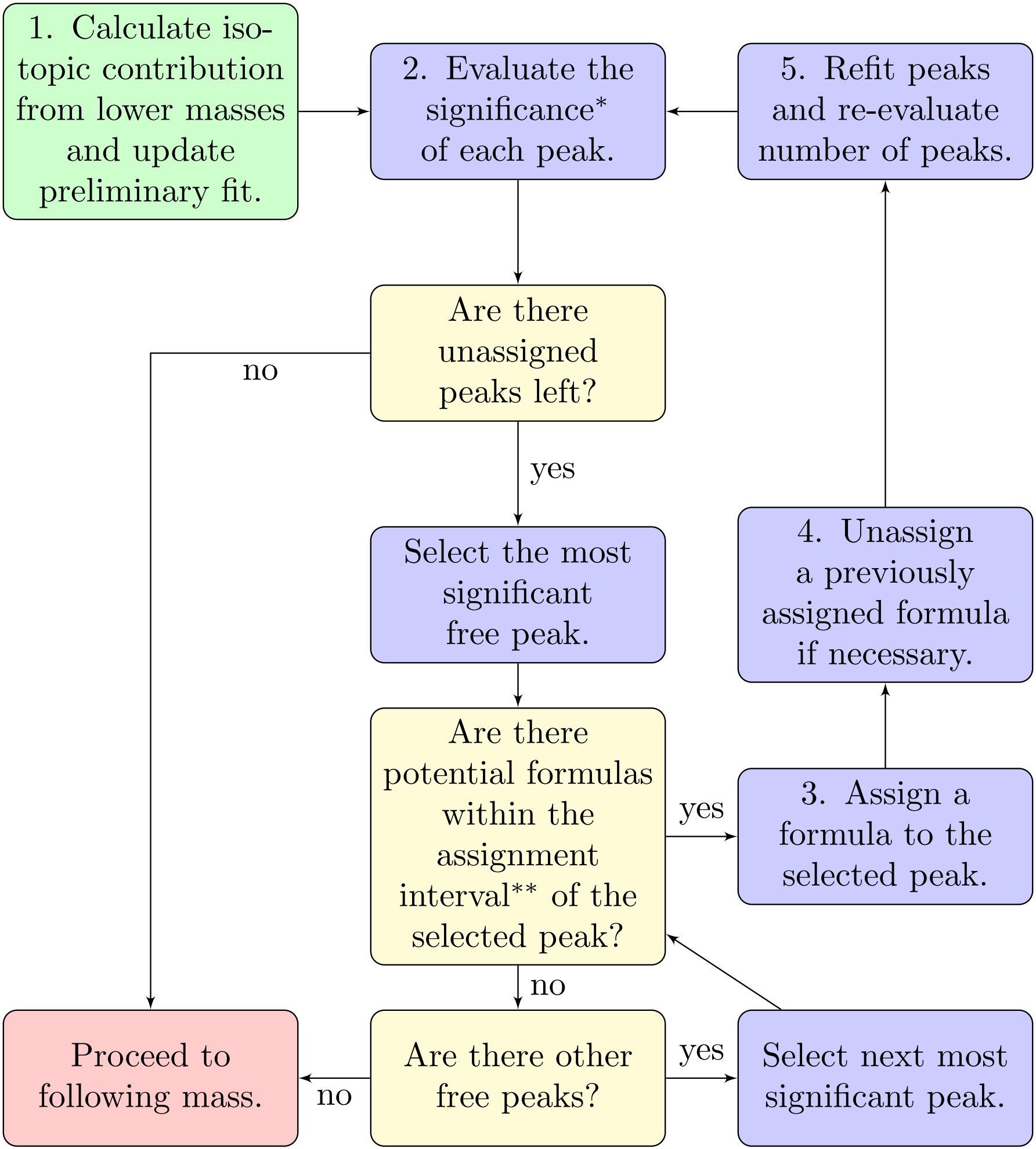
1. Calculate isotopic contribution from lower masses and update preliminary fit.
2. Evaluate the significance* of each peak.
5. Refit peaks and re-evaluate number of peaks.
Are there unassigned peaks left?
no
yes
Select the most significant free peak.
4. Unassign a previously assigned formula if necessary.
Are there potential formulas within the assignment interval** of the selected peak?
yes
3. Assign a formula to the selected peak.
no
Proceed to following mass.
Are there other free peaks?
yes
Select next most significant peak.
no